607. DECHEMA Colloquium, 26.10.2006, Frankfurt/Main

New horizons for diffusion research in nanoporous materials: Experiments, Theory and Application.

Diffusion in zeolites – a never-ending story?

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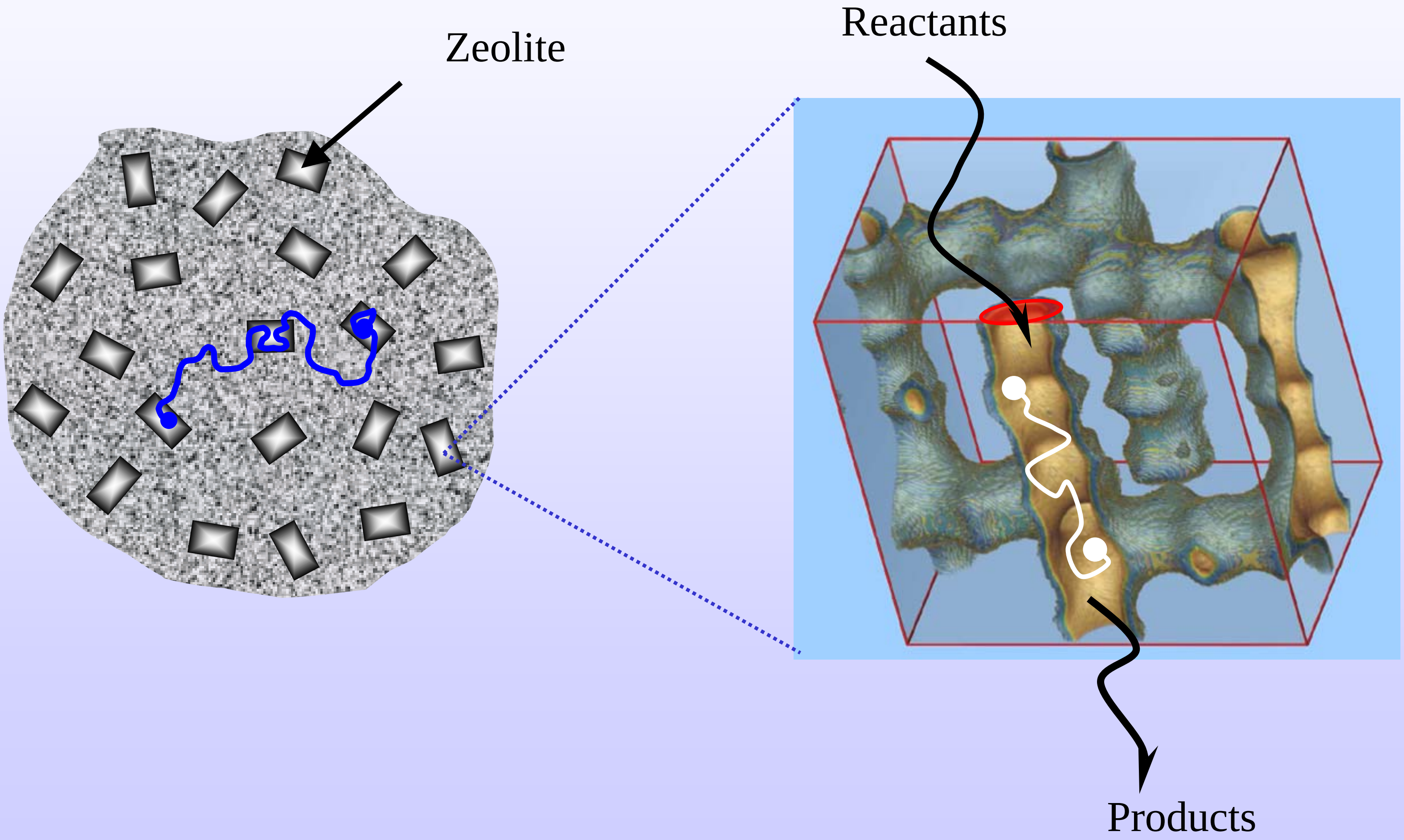
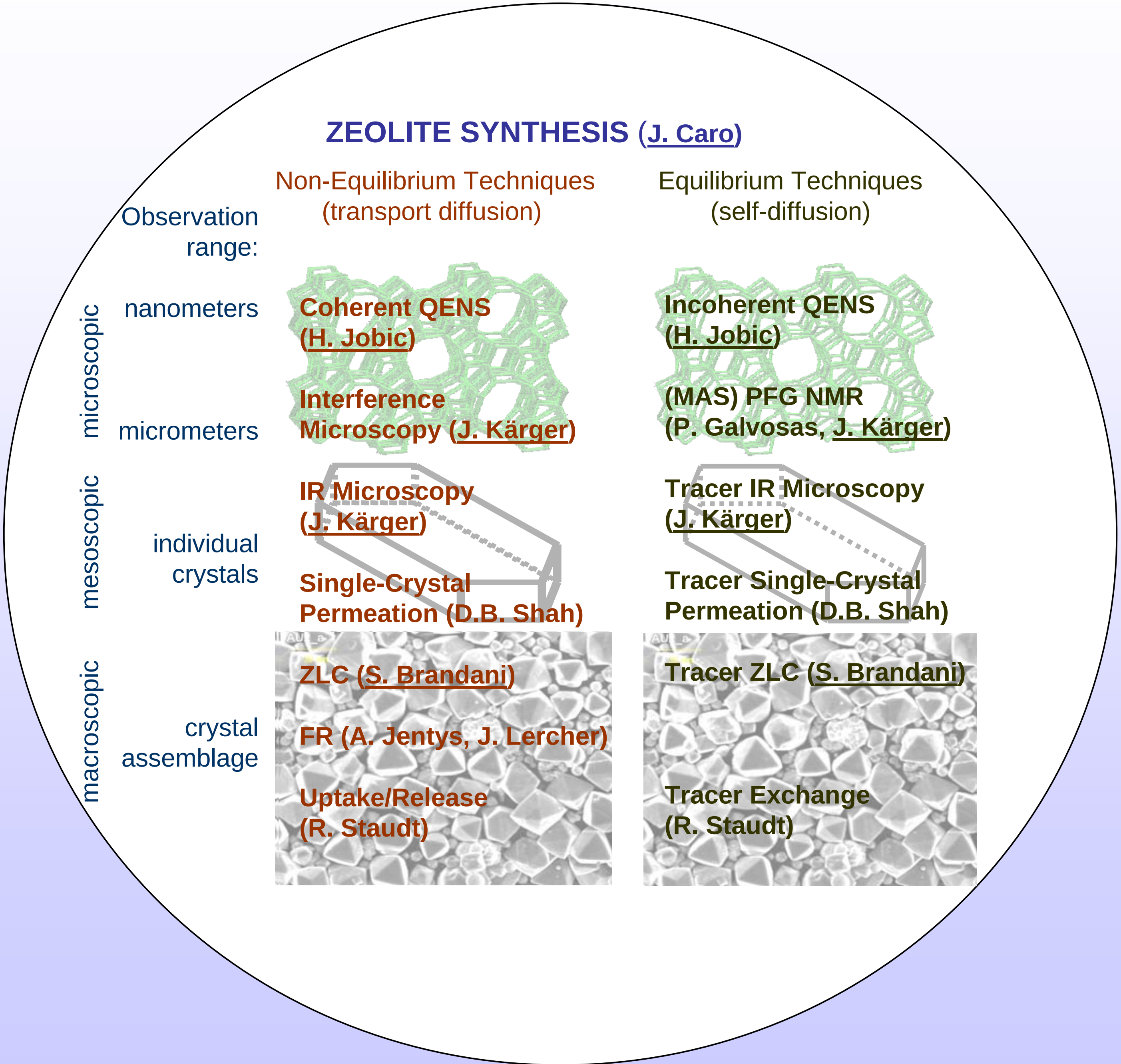
Economic motivation of our activities in technical application



Package of Research Projects **"Diffusion in Zeolites"**

by CNRS (France), DFG (Germany), EPSRC (United Kingdom), NSF (USA)

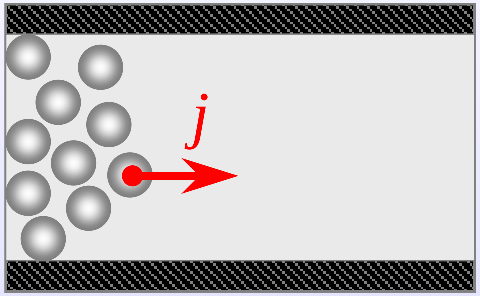


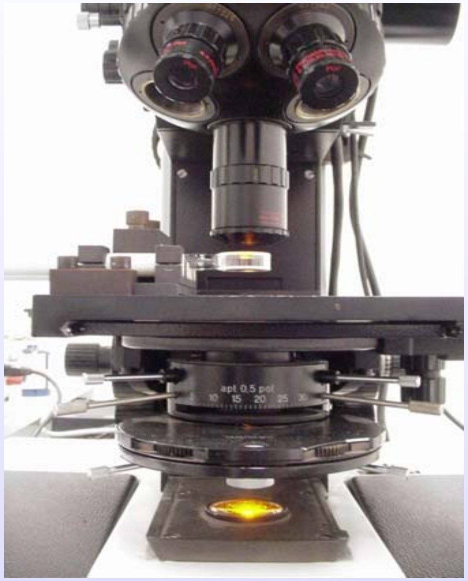
What do we measure?

Interference Microscopy (IFM)

$$j = -D_{(T)}\ \mathrm{grad}\ c$$

transport diffusion

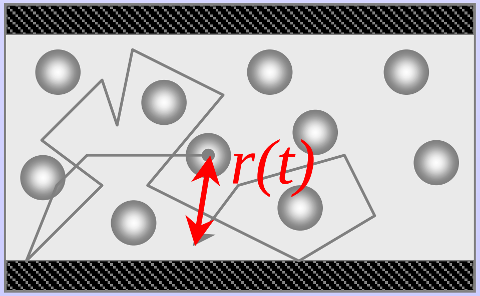




Pulsed Field Gradient (PFG) NMR

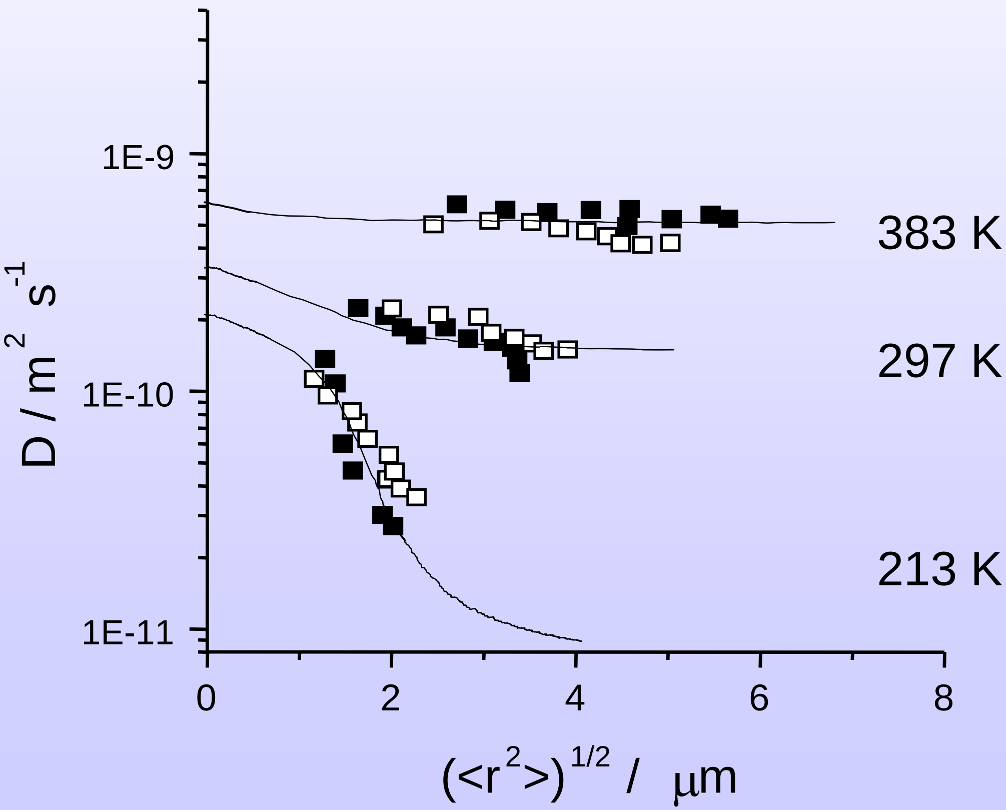
$$\langle r^2(t)\rangle = 2D\,t$$

self-diffusion



Intracrystalline Diffusion

Comparison of the PFG NMR results with the results of MC simulations



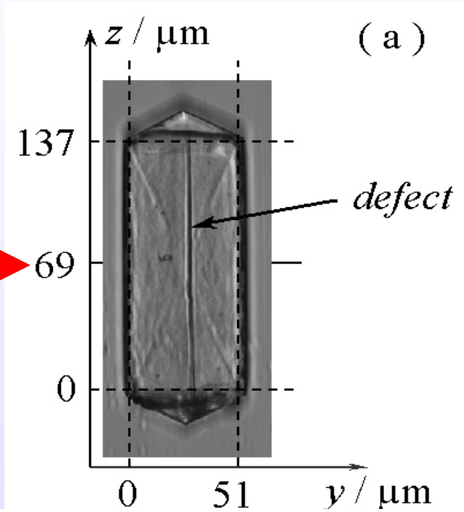
n-Butane / Silicalite-1

two sets of measurement with different samples

$p_y = 1$ $p_x = 0.32$
$p_z = 0.067$ [1]

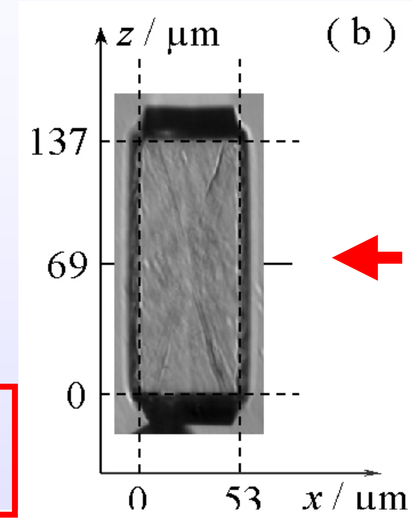
$(E_b - E_d) = 21.5$ kJ/mol
N = 3000 (×1nm)

Interference Microscopy (IFM): Influence of defects on the external crystal surface on the isobutane uptake into MFI-type zeolite

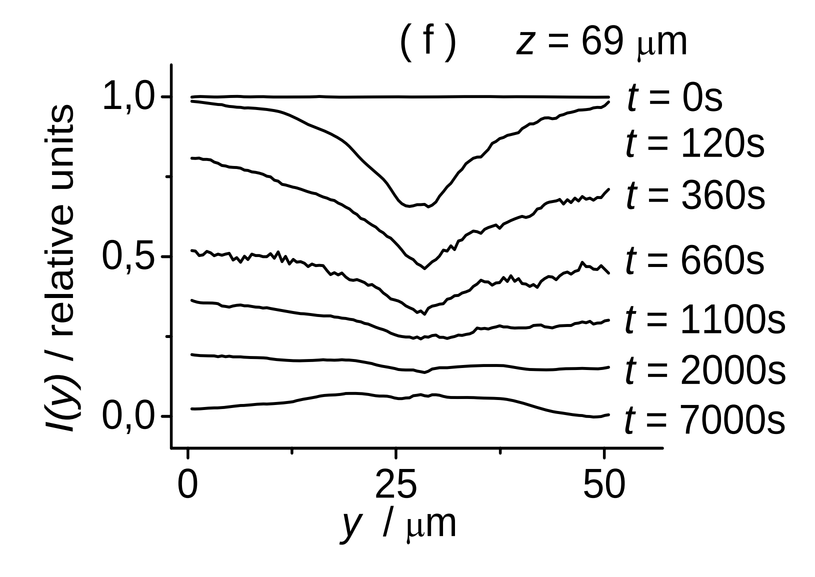


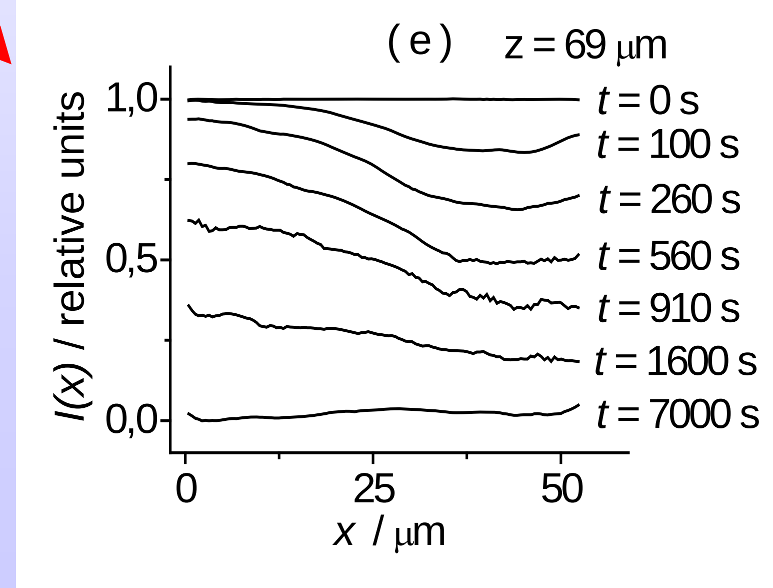
The non-etched sample (strong surface barriers)

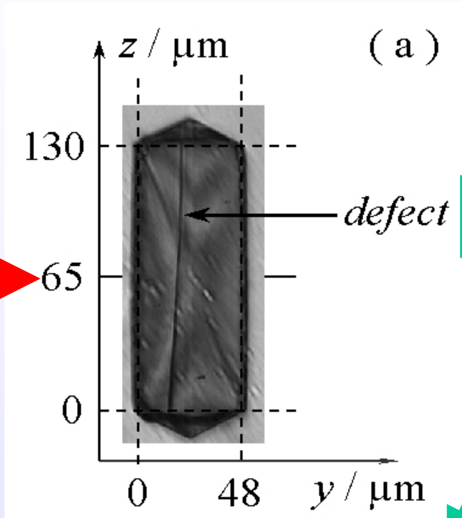
Faster desorption in the middle part of the crystals than near crystal edges: desorption through the crack surface



Faster desorption in the crystal part with the crack



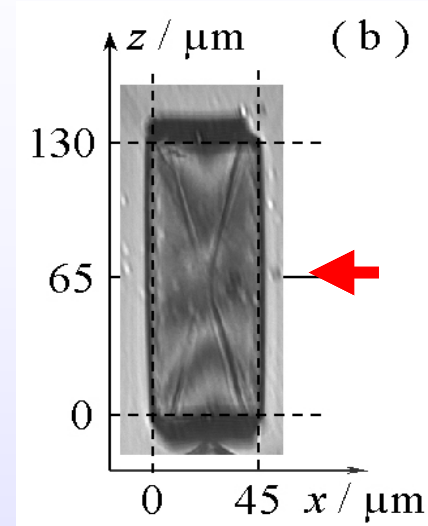


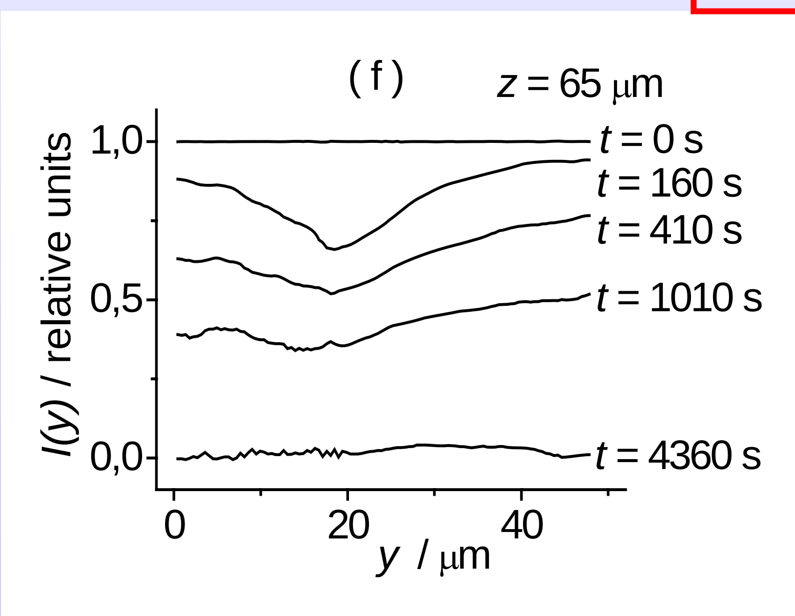


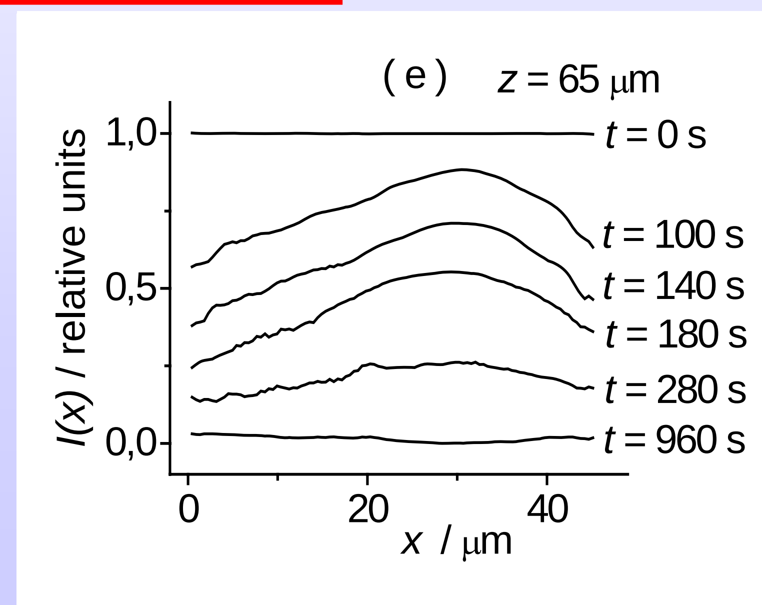
The etched sample (mild surface barriers)

Desorption through the crack surface

(i) Both the diffusivity and permeability of transport barriers determine the rate of desorption
(ii) Faster desorption in the crystal part with the crack







Physical

~~Medical~~ diagnosis has attained such a high level

perfect crystal

that there scarcely exist any really ~~healthy people~~.

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• Diffusion in zeolites – a never-ending story?
Prof. ***J. Kärger***, Universität Leipzig

• Diffusion studies by QENS – measurements apporaching the „ideal“ situation
Dr. ***H. Jobic***, Institut de Rechsrches sur la Catalyse, Villeurbanne, France

• Correlating molecular modelling and experimental diffusivities
Prof: ***D. Theodorou***, National Technical University of Athens, Greece

• Ideal vs. Real zeolite structure: options to discriminate
Prof. ***J. Caro***, Universität Hannover

• Studying „macroscopic“ aspects of diffusion
Prof. ***S. Brandani***, University College London

• From diffusion research to industrial application
Prof. ***D. Ruthven***, University of Maine, Orono, Maine, USA

• Mass transfer coefficients determined from break-through experiments
Dr. ***J. Oppermann***, Linde AG, Höllriegelskreuth